

Exact Keldysh theory of strong-field ionization: residue method vs saddle-point approximation

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In recent articles [Mishima *et al.*, Phys. Rev. A, **66**, 033401 (2002); Chao, Phys. Rev. A, **72**, 053414 (2005)] it was proposed to use the residue theorem for the exact calculation of the transition amplitude describing strong-field ionization of atomic systems within Keldysh theory. This should avoid the necessity to apply the method of steepest descent (saddle-point approximation). Comparing the results of both approaches for atomic hydrogen a difference by a factor of 2 was found for the 1s, and an even more drastic deviation for the 2s state. Thus it was concluded that the use of the saddle-point approximation is problematic. In this work the deviations are explained and it is shown that the previous conclusion is based on an unjustified neglect of an important contribution occurring in the application of the residue theorem. Furthermore, the applicability of the method of steepest descent for the ionization of Rydberg states is discussed and an improvement of the standard result is suggested that successfully removes the otherwise drastic failure for large principal quantum numbers.

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I. INTRODUCTION

The ionization process in atomic systems exposed to a strong laser field has attracted great interest during the past decades and its proper modeling remains a challenge to theory [1]. Among the numerous approximations developed to treat this problem Keldysh theory [2] possesses a prominent role. This theory was proposed by Keldysh 40 years ago and describes the ionization process as a transition between an initial electronic bound and a Volkov continuum state (adopting the length gauge formulation). Besides the main approximation of the Keldysh theory, the neglect of the interaction of the escaping electron with the long-range Coulomb potential (in the case of a neutral atom), two additional simplifications were made in [2]: (i) the method of steepest descent (MSD) [3] (saddle-point approximation) for performing an occurring contour integral, and (ii) the assumption of a small kinetic momentum of the escaping electron. The Keldysh approximation and variants of it are also very popular, because they are the basis for methods that predict strong-field ionization rates also for heavier atoms and molecules (see, e. g., [4, 5]).

Recently, there has been proposals to obtain an exact Keldysh theory by removing the two additional simplifications (i) and (ii). It was especially suggested to avoid approximation (i) by solving the occurring contour integrals with the aid of the exact residue theorem (RT) instead of the MSD [6, 7, 8]. It was shown that the RT method yields a two times larger transition amplitude for the 1s state of a hydrogen-like atom and, as a consequence, a four times larger ionization rate. Furthermore, the ionization rate of the first excited (2s) state obtained in [8] when applying the RT differs significantly from the MSD result. In view of the popularity of the MSD approximation for treating strong-field problems like ionization [9] or high-harmonic generation [10] this is of course

a very important result. This has motivated the present study in which a careful reinvestigation of the RT and the MSD is performed (Sec. II). It is shown that the application of the RT as proposed in [6, 7, 8] contains an unjustified neglect of the contribution of one integral and that it is this omission which is the main source for the previously reported deviation between the RT and the MSD results. Therefore, the MSD provides in fact more reliable results than the (incomplete) RT approach. It is furthermore discussed that the MSD fails for Rydberg states and a correction to it is proposed. The conclusions of Sec. II are supported with the aid of a numerical study in Sec. III.

II. THEORY

A. Transition amplitude

In order to provide the basis for the subsequent discussion and to introduce the notation a brief summary of the Keldysh theory is given that follows closely the one described in Appendix A of [11]. The total ionization rate of a one-electron atomic system with the electron binding energy E_b in the harmonic laser field $\mathbf{F}(t) = \mathbf{F} \cos \omega t$, with the period $T = 2\pi/\omega$, can be expressed as the sum over N -photon processes (atomic units are used throughout this work)

$$W = 2\pi \int \frac{d^3p}{(2\pi)^3} |A(\mathbf{p})|^2 \sum_{N=N_{\min}}^{\infty} \delta(E_b + \frac{p^2}{2} + U_p - N\omega) \quad (1)$$

where $U_p = F^2/(4\omega^2)$ is the electron quiver (ponderomotive) energy due to the field. The transition amplitude

$A(\mathbf{p})$ can be calculated using

$$A(\mathbf{p}) = \frac{1}{T} \int_0^T dt \int d^3r \Psi_{\mathbf{p}}^*(\mathbf{r}, t) V_F(t) \Psi_0(\mathbf{r}, t) \quad (2)$$

where $\Psi_0(\mathbf{r}, t) = e^{iE_b t} \Phi_0(\mathbf{r})$ is the wave function describing the initial electronic state in the atomic potential $U(\mathbf{r})$. Therefore, $\Phi_0(\mathbf{r})$ fulfills the stationary Schrödinger equation

$$\left[-\frac{1}{2} \nabla^2 + U(\mathbf{r}) + E_b \right] \Phi_0(\mathbf{r}) = 0 \quad (3)$$

The interaction with the laser field is given in length gauge by $V_F(t) = \mathbf{r} \cdot \mathbf{F}(t)$. Finally, the Volkov wave function [12] $\Psi_{\mathbf{p}}(\mathbf{r}, t)$ satisfies

$$i \frac{\partial \Psi_{\mathbf{p}}}{\partial t} = \left[-\frac{1}{2} \nabla^2 + V_F(t) \right] \Psi_{\mathbf{p}}, \quad (4)$$

and can be explicitly written as

$$\Psi_{\mathbf{p}}(\mathbf{r}, t) = \exp \left[i \mathbf{r} \cdot \boldsymbol{\pi}(t) - \frac{i}{2} \int_0^t \pi^2(t') dt' \right] \quad (5)$$

where $\boldsymbol{\pi}(t) = \mathbf{p} + (\mathbf{F}/\omega) \sin \omega t$ is the mechanical momentum of an electron with the canonical momentum \mathbf{p} in the field $\mathbf{F}(t)$. Introducing the auxiliary functions

$$V_0(\mathbf{q}) = \int d^3r e^{-i\mathbf{q} \cdot \mathbf{r}} (\mathbf{F} \cdot \mathbf{r}) \Phi_0(\mathbf{r}) = i \mathbf{F} \cdot \nabla_{\mathbf{q}} \tilde{\Phi}_0(\mathbf{q}) \quad (6)$$

(where $\tilde{\Phi}_0(\mathbf{q})$ is the Fourier transform of $\Phi_0(\mathbf{r})$) and

$$S(t) = \int_0^t dt' \left[E_b + \frac{1}{2} \pi^2(t') \right] \quad (7)$$

the transition amplitude $A(\mathbf{p})$ can be rewritten as

$$A(\mathbf{p}) = \frac{1}{T} \int_0^T dt \cos(\omega t) V_0(\boldsymbol{\pi}(t)) e^{iS(t)} \quad (8)$$

The equivalence of $A(\mathbf{p})$ in (8) and $L(\mathbf{p})$ in Eq. (15) of the original Keldysh work [2] can be shown in the following way. The path of the integration over t in (8) can be shifted into the complex plane by means of the transformation $\tilde{t} = t + i\epsilon$ where ϵ is an infinitesimally small positive number. Introduction of the new complex variable $u = \sin \omega \tilde{t} = \sin \omega t + i\epsilon \cos \omega t$ transforms the integration $\int_0^T dt$ to one on the closed contour C_{in} which encloses the interval $(-1, 1)$ (see Fig. 1 a). Applying the same procedure to the integral contained in the function $S(t)$ yields

$$A(\mathbf{p}) = \oint_{C_{\text{in}}} du \tilde{V}_0(u) e^{iS(u)} \quad (9)$$

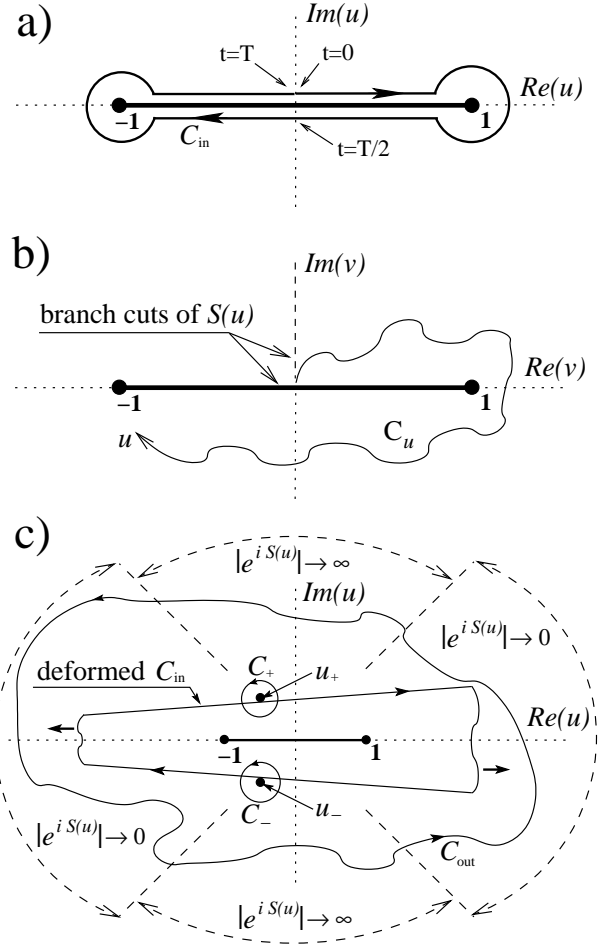


FIG. 1: (a) The path C_{in} of the contour integration for $A(\mathbf{p})$. (b) The path C_u of the contour integration for $S(u)$. (c) The asymptotic behavior of $\exp[iS(u)]$, contours C_{\pm} around saddle points u_{\pm} , contour C_{out} , and deformed C_{in} used within MSD.

where

$$\tilde{V}_0(u) = \frac{1}{2\pi} V_0 \left(\mathbf{p} + \frac{\mathbf{F}}{\omega} u \right) \quad (10)$$

$$S(u) = \int_{C_u} \frac{dv}{f(v)} \left[\frac{E_b}{\omega} + \frac{1}{2\omega} \left(\mathbf{p} + \frac{\mathbf{F}}{\omega} v \right)^2 \right]. \quad (11)$$

The transition amplitude $A(\mathbf{p})$ in (9) is for $f(v) = \sqrt{1-v^2}$ identical to $L(\mathbf{p})$ in [2] which is also the starting point of the analysis in [6]. Since the square root is usually defined to possess a non-negative real part which can in the present context be misleading and cause a sign error, we introduce the function

$$f(v) = \text{Sign}[\text{Im}(v)] \sqrt{1-v^2}, \quad (12)$$

which is analytical in the whole complex plane except its branch cut $[-1, 1]$. The path of integration C_u specifies the clockwise path around the branch cut (see Fig. 1 b)

starting at $v = i\epsilon$ and terminating at $v = u$. Note, $S(u)$ is a multivalued function, so we have selected also the branch cut along positive imaginary axis.

Due to the delta function in Eq.(1) one needs to calculate $A(\mathbf{p})$ only for $|\mathbf{p}| = p_N = \sqrt{2(N\omega - E_b - U_p)}$. Both (8) and (9) can equivalently be used for numerical integration to yield an exact result. The use of (9) provides more flexibility, since the contour C_{in} can be deformed in a convenient way.

There exist two special points u_{\pm} (A4) in the complex plane u . They are simultaneously the saddle points of $S(u)$ and poles of $\tilde{V}_0(u)$. In [2] Keldysh has used MSD to approximate $A(\mathbf{p})$. In [6] the authors have proposed to use RT [3] for an exact calculation of $A(\mathbf{p})$. For the 1s state of hydrogen-like atoms the expression for $A(\mathbf{p})$ obtained in [6] is larger than that of Keldysh using MSD by exactly a factor of two, provided the small \mathbf{p} approximation is consistently used or omitted in both the RT and the MSD approach. As is shown below, the disagreement is a consequence of a wrong assumption made in [6]. In fact, for excited states of hydrogen-like atoms the therein proposed approach may lead to drastically wrong results.

For spherically symmetric bound states of hydrogen-like atoms with principal quantum number n the function $\tilde{V}_0(u)$ can be presented (see Appendix B) as

$$\tilde{V}_0(u) = \frac{g_+(u)}{(u - u_+)^{\nu}} = \frac{g_-(u)}{(u - u_-)^{\nu}}, \quad \nu = n + 2 \quad (13)$$

where $g_{\pm}(u) = \tilde{V}_0(u)(u - u_{\pm})^{\nu}$ is an analytical (and, possibly, slowly varying) function in the vicinity of the special points u_{\pm} . Both procedures (MSD and RT) are considered in this work for general $\tilde{V}_0(u)$ having poles of order ν at $u = u_{\pm}$.

B. The residue theorem

Since for $|\mathbf{p}| = p_N$ the function $\tilde{V}_0(u) \exp[iS(u)]$ is analytical in the whole complex plane except the branch cut $[-1, 1]$ and the poles u_{\pm} , (9) can be modified using

$$\oint_{C_{\text{in}}} = \oint_{C_+} + \oint_{C_-} - \oint_{C_{\text{out}}} \quad (14)$$

where C_{\pm} are contours around u_{\pm} and C_{out} is a contour enclosing $(-1, 1)$ and u_{\pm} (see Fig. 1 c). The integrals A_{\pm} along C_{\pm} can be calculated using RT which yields

$$A_{\pm} = \frac{2\pi i}{(\nu - 1)!} \lim_{u \rightarrow u_{\pm}} \frac{d^{\nu-1}}{du^{\nu-1}} [g_{\pm}(u) e^{iS(u)}] \quad (15)$$

With the knowledge of the integral along C_{out} ,

$$I_{\text{out}} = \oint_{C_{\text{out}}} du \tilde{V}_0(u) e^{iS(u)}, \quad (16)$$

the value of $A(\mathbf{p})$ can be calculated using (14) as

$$A(\mathbf{p}) = (A_+ + A_-) - I_{\text{out}}. \quad (17)$$

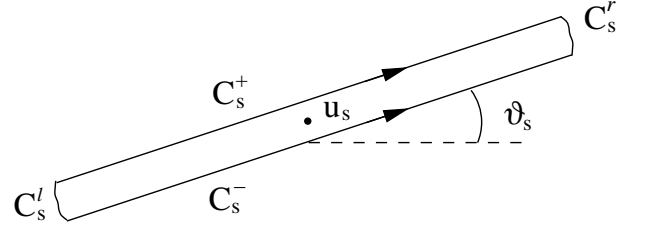


FIG. 2: The integration paths C_s^{\pm} passing around the special point u_s from both sides and given parametrically in Eq.(20). The contours C_s^r and C_s^l are used to connect the contours C_s^{\pm} at infinity.

In [6] the value of I_{out} is implicitly assumed to be zero. However, a simple analysis shows that there are no reasons for such an assumption. Indeed, for $u = Re^{i\theta}$ with $R \rightarrow \infty$, one finds [see Eq. (A2)]

$$e^{iS(u)} \rightarrow e^{-(U_p/\omega)R^2 \cos(2\theta)} e^{-(U_p/\omega)R^2 \sin(2\theta)i}. \quad (18)$$

Since $\tilde{V}_0(u) \sim R^{-5}$ for $R \rightarrow \infty$, the integrand in (16) has the following limits:

$$\begin{aligned} |\tilde{V}_0(u) e^{iS(u)}| &\rightarrow 0, & -\frac{\pi}{4} < \theta < \frac{\pi}{4}, & \frac{3\pi}{4} < \theta < \frac{5\pi}{4}, \\ |\tilde{V}_0(u) e^{iS(u)}| &\rightarrow \infty, & -\frac{3\pi}{4} < \theta < -\frac{\pi}{4}, & \frac{\pi}{4} < \theta < \frac{3\pi}{4}. \end{aligned}$$

Therefore, it is impossible to select C_{out} in such a way that the integrand on the whole contour approaches zero. Moreover, in section III it is numerically demonstrated that I_{out} is of the same order of magnitude as $A(\mathbf{p})$ or even larger.

C. Contours through steepest descent

In order to understand the appearance of the factor two between the RT and the MSD results it is important to connect the two approaches. For this purpose, the four auxiliary integrals

$$I_s^{\pm} = \int_{C_s^{\pm}} g_s(u) \frac{e^{iS(u)}}{(u - u_s)^{\nu}} du \quad (19)$$

are introduced where the index $s = \pm$ specifies one of the two special points. The contours C_s^{\pm} are given parametrically by

$$u_x = u_s + (x \pm i\epsilon) Q_s, \quad -\infty < x < \infty, \quad \epsilon \rightarrow 0^+ \quad (20)$$

starting at $x \rightarrow -\infty$. Here, plus (minus) corresponds to the contour passing slightly above (below) the special point u_s (see Fig. 2). The value of Q_s is chosen in such a way that the contours C_s^{\pm} are passing through the steepest descent of $iS(u)$, i.e. as

$$Q_s = \sqrt{\frac{2i}{S''(u_s)}} \quad (21)$$

where the argument Q_s satisfies $-\pi/4 < \arg Q_s < \pi/4$ (see Eqs.(A8)). According to (18) the integrand in (19) must then exponentially decay to 0 for $x \rightarrow \pm\infty$. This specific choice of Q_s allows to directly apply MSD in the following subsection. Here, Cauchy integration rules [3] are employed to deduce three useful relations:

- (i) Deforming the contour in $A(\mathbf{p})$ to pass along C_-^+ in positive direction, along C_+^- in negative direction and connecting the ends of these contours at infinity one obtains

$$A(\mathbf{p}) = I_+^- - I_-^+ \quad . \quad (22)$$

- (ii) Connecting contours C_s^\pm at infinity with the contours C_s^l and C_s^r (see Fig. 2) and applying the residue theorem one obtains

$$A_s = I_s^- - I_s^+ \quad . \quad (23)$$

- (iii) Substituting (22) and (23) into (17) one obtains

$$I_{\text{out}} = I_-^- - I_+^+ \quad . \quad (24)$$

Note, the use of a sufficiently small but finite positive ε yields the same value of I_s^\pm . This is used to compute I_s^\pm numerically.

Keeping in mind that equations (22), (23), and (24) are exact and no approximations have been done so far, we apply now MSD to approximate I_s^\pm .

D. The method of steepest descent in the presence of a singularity

Since no difference is made between two different contour integrations around the same saddle point (as, e. g., for I_s^+ and I_s^-) in [11] (Appendix B), we shortly repeat the main steps. From (20) the relations

$$du = Q_s dx, \quad \frac{1}{(u_x - u_s)^\nu} = \frac{(\pm 1)^\nu}{(iQ_s)^\nu} \frac{1}{(\epsilon \mp ix)^\nu} \quad (25)$$

follow. We expect the vicinity of u_s to give the main contribution to the integral and assume that $g_s(u)$ is a slowly varying function in the vicinity of u_s . Then, using the approximation

$$g_s(u)e^{iS(u_x)} \approx g_s(u_s)e^{iS(u_s)}e^{-x^2 \mp 2i\epsilon x + \epsilon^2} \quad (26)$$

and the identity

$$\frac{1}{(a \mp ib)^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty d\eta \eta^{\nu-1} e^{-\eta a} e^{\pm i\eta b}, \quad a > 0 \quad (27)$$

one obtains

$$\begin{aligned} I_s^\pm &\approx (\pm 1)^\nu \frac{g_s(u_s)e^{iS(u_s)}}{i^\nu Q_s^{\nu-1} \Gamma(\nu)} \int_0^\infty d\eta \eta^{\nu-1} e^{-\eta\epsilon + \epsilon^2} \\ &\times \int_{-\infty}^\infty dx e^{-x^2 \pm i(\eta-2\epsilon)x}. \end{aligned} \quad (28)$$

The integration over x and η yields

$$I_s^\pm \approx (\pm 1)^\nu I_s, \quad I_s = \frac{\pi g_s(u_s) e^{iS(u_s)}}{i^\nu Q_s^{\nu-1} \Gamma(\frac{\nu+1}{2})}. \quad (29)$$

Therefore, MSD predicts I_s^\pm to be equal for even ν and to differ only by the sign for odd ν . Using equations (22) and (24) this result can be rewritten as

$$I_{\text{out}} = (-1)^{\nu-1} A(\mathbf{p}) \quad [\text{within MSD}]. \quad (30)$$

Using (22) the prediction of MSD for $A(\mathbf{p})$ is

$$A_{\text{MSD}} = (-1)^\nu I_+ - I_- \quad . \quad (31)$$

Substitution of (30) into (17) shows that for odd ν MSD yields

$$A(\mathbf{p}) \approx (A_+ + A_-)/2 \quad [\text{MSD, odd } \nu]. \quad (32)$$

Its value is thus two times smaller than the one obtained with the assumption $I_{\text{out}} = 0$. For even ν MSD predicts

$$|A(\mathbf{p})| \gg |(A_+ + A_-)| \quad [\text{MSD, even } \nu]. \quad (33)$$

Note, (32) and (33) are valid for every $\tilde{V}_0(u)$ satisfying (13), if $g_\pm(u)$ is a slowly varying function in the vicinity of u_\pm . The fact that for the 1s state of hydrogen-like atoms ($\nu = 3$) one finds exactly a factor 2 difference between MSD and RT and thus an equality sign in (32) should be seen as an accidental case that is due to the relative simplicity of $\tilde{V}_0(u)$ for the 1s state.

In section III MSD is tested numerically and it is shown that the assumption of a slowly varying function $g_\pm(u)$ is valid only for small n (or ν).

III. NUMERICAL TEST

To support our conclusions of the previous section the example results of a numerical study are reported in Table I. For a more transparent analysis a number of parameters were fixed. This includes the amplitude of the electric field $\mathbf{F} = 0.02$ a.u., the frequency $\omega = 0.01$ a.u., the binding energy $E_b = Z^2/(2n^2) = 0.5$ a.u. (thus charge $Z = n$), the angle $\hat{\mathbf{F}} \cdot \hat{\mathbf{p}} = 0.9$, and the number of photons $N = 161$. With such a choice of fixed parameters a variation of the principal quantum number n leaves the function $S(u)$ unchanged (see Appendix A for details). The same is true for the positions of the special points u_\pm and the values of Q_\pm . Therefore, only function $\tilde{V}_0(u)$ varies with n .

We use (8) to calculate the exact value A_{ex} of $A(\mathbf{p})$ and (15) to evaluate A_\pm . The integrals I_s^\pm are calculated numerically, Eq.(22) and (23) are used for a check of the numerics and I_{out} is obtained from (24).

As follows from the discussion above, the condition $I_s^- \approx (-1)^\nu I_s^+$ obtained in (29) can be used as a criterion for the validity of the simple MSD formula (31).

TABLE I: Contour integrals I_{\pm}^{\pm} , I_{\pm}^{-} [Eq.(19)], I_{out} [Eq.(24)], quantities I_{\pm} [Eq.(29)], and $A_{+} + A_{-}$ [Eq.(15)] for different principal quantum numbers n and fixed parameters ($F = 0.02$ a. u., $\omega = 0.01$ a. u., $E_b = 0.5$ a. u., $\hat{\mathbf{F}} \cdot \hat{\mathbf{p}} = 0.9$, $N = 161$). The exact value A_{ex} for the amplitude $A(\mathbf{p})$ [Eq.(8)] is compared with the prediction of the simple MSD formula A_{MSD} [Eq.(31)], the corrected MSD formula A_{cMSD} [Eq.(C5)], and the amplitude A_{KM} (with appropriate phase normalization) given by the “two-term saddle-point approximation” [13].

	$n = 1, \times 10^{-8}$	$n = 2, \times 10^{-7}$	$n = 3, \times 10^{-6}$	$n = 4, \times 10^{-5}$	$n = 5, \times 10^{-4}$
I_{+}^{+}	$-0.212 - 1.560 i$	$-0.320 - 1.760 i$	$-0.374 - 1.652 i$	$-0.371 - 1.370 i$	$-0.326 - 1.034 i$
I_{+}^{-}	$0.226 + 1.883 i$	$-0.302 - 1.884 i$	$0.274 + 1.347 i$	$-0.189 - 0.758 i$	$0.105 + 0.352 i$
I_{-}^{+}	$-0.219 - 1.722 i$	$-0.312 - 1.812 i$	$-0.325 - 1.495 i$	$-0.276 - 1.045 i$	$-0.201 - 0.644 i$
I_{-}^{-}	$-1.180 - 1.485 i$	$1.127 + 1.539 i$	$-0.765 - 1.142 i$	$0.406 + 0.667 i$	$-0.176 - 0.322 i$
I_{+}^{+}	$0.960 + 1.248 i$	$1.027 + 1.465 i$	$0.912 + 1.428 i$	$0.713 + 1.227 i$	$0.506 + 0.959 i$
I_{-}^{-}	$-1.070 - 1.366 i$	$1.069 + 1.496 i$	$-0.835 - 1.282 i$	$0.549 + 0.931 i$	$-0.317 - 0.595 i$
$A_{-} + A_{+}$	$2.578 + 6.175 i$	$-0.083 - 0.199 i$	$2.325 + 5.569 i$	$0.490 + 1.172 i$	$1.113 + 2.666 i$
I_{out}	$1.172 + 2.808 i$	$1.346 + 3.224 i$	$1.286 + 3.080 i$	$1.084 + 2.597 i$	$0.832 + 1.993 i$
A_{MSD}	$1.289 + 3.088 i$	$-1.381 - 3.308 i$	$1.160 + 2.778 i$	$-0.825 - 1.976 i$	$0.517 + 1.239 i$
A_{cMSD}	$1.406 + 3.367 i$	$-1.432 - 3.431 i$	$1.047 + 2.506 i$	$-0.603 - 1.444 i$	$0.287 + 0.687 i$
A_{ex}	$1.406 + 3.368 i$	$-1.429 - 3.423 i$	$1.039 + 2.489 i$	$-0.595 - 1.425 i$	$0.281 + 0.673 i$
A_{KM}	$1.378 + 3.300 i$	$-1.680 - 4.025 i$	$1.641 + 3.932 i$	$-1.365 - 3.270 i$	$0.999 + 2.393 i$

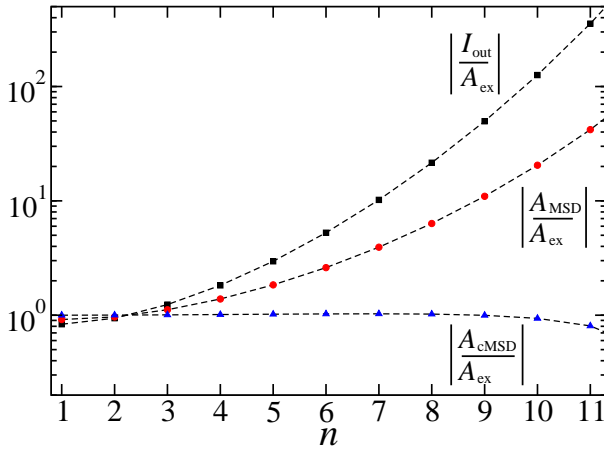


FIG. 3: (Color online) Demonstration of the failure of the MSD for large principal quantum numbers n . The ratio $|I_{\text{out}}/A_{\text{ex}}|$ (boxes) grows exponentially with n which causes an increase of the ratio $|A_{\text{MSD}}/A_{\text{ex}}|$ (circles) between the approximate and exact amplitudes A_{MSD} and A_{ex} , respectively. Therefore, the simple (standard) MSD formula [Eq.(31)] fails and must be improved to be applicable for large n . The in this work proposed corrected MSD formula [Eq.(C5)] shows very good accuracy in a large region of n , as can be seen from the corresponding ratio $|A_{\text{cMSD}}/A_{\text{ex}}|$ (triangles). The parameters used in the computation are the same as in Table I.

Table I shows that this condition is fulfilled for $n = 1, 2$ and the relations (30,32,33) are valid. With increasing n the condition is, however, not well fulfilled and the accuracy of the MSD prediction decreases. Numerical tests show that for large n the values $|I_{+}^{+}|, |I_{-}^{-}|$ are by orders of magnitude larger than $|I_{+}^{-}|, |I_{-}^{+}|$. This leads to the

following relations (see Fig. 3)

$$|A_{\text{ex}}| \ll |A_{\text{MSD}}|, \quad |A_{\text{ex}}| \ll |I_{\text{out}}|, \quad I_{\text{out}} \approx A_{+} + A_{-}.$$

Therefore, function $\tilde{V}_0(u)$ cannot be given as simple as in (13). Instead, $\tilde{V}_0(u)$ can be represented in the vicinity of u_s by a sum over terms having different orders of poles (see Eq.(B7)). Moreover, it is possible to consider also higher derivatives of $S(u)$, as is done in Eq.(C2). The resulting representation of $\tilde{V}_0(u) \exp[iS(u)]$ given in Eq.(C3) and the subsequent use of MSD to it leads to a much higher accuracy. As can be seen from Table I and Fig. 3 the corrected MSD formula (C5) yields a significant improvement and can be used for the numerical computation of $A(\mathbf{p})$ in a large range of n . This paves the way for a detailed study of the validity of the Keldysh approximation for, e. g., Rydberg atoms that is not blurred by a failure of the usually adopted MSD approximation.

It is instructive to compare A_{cMSD} with the recently published “two-term saddle-point approximation” [13]. This approximation is a modification of the “one-term saddle-point approximation” [11]. Both approximations are based on the principle that only the leading term of the Laurent expansion of the Fourier transform $\hat{\Phi}_0(\mathbf{q})$ at the saddle points is considered. Since in the “one-term” approximation the contributions from higher-order derivatives of $S(u)$ are also ignored, it is equivalent to the simple MSD formula A_{MSD} and yields thus the same numerical results. (Note, the resulting expressions are, however, different, because different complex variables $\phi = \omega t$ and u are used in the derivations.) As can be seen from Table I, the amplitude A_{KM} yielded by the “two-term” approximation (using an appropriate phase normalization) gives relatively good agreement for $n = 1$, although it is clearly less accurate than A_{cMSD} . For the

excited states the “two-term” formula fails rapidly and yields results which are even less accurate than the ones obtained with the “one-term” formula. To understand this fact, we remind that the second term in [13] comes from the next-to-leading pole, and only the contribution arising from the third derivative of $S(u)$ is considered. A detailed analysis shows that a singularity of the same order can also arise from the next-to-leading term of the Laurent expansion of $\tilde{\Phi}_0(\mathbf{q})$. In addition, for larger values of n it can also be important to consider further terms of the Laurent expansion. Since the corrected MSD formula (C5) takes all of this into account, the resulting A_{cMSD} is significantly more accurate than A_{KM} .

IV. CONCLUSION

In this work it has been demonstrated that the residue theorem was not correctly employed in [6, 7], since the derivation was based on an unjustified assumption that one integral vanishes. This neglected term is, however, of the same order of magnitude as the remaining ones or even much larger. For the 1s state of hydrogen-like atoms it is almost identical, and thus its omission results in an overestimation of the transition amplitude by a factor two for this case. This deviation was in [6] incorrectly assumed to be a failure of the widely used saddle-point approximation. Considering a 2s state, it is furthermore concluded that an application of the method proposed in [6] to a 2s state would yield an even larger (erroneous) deviation.

Such a large deviation for the 2s state was in fact reported in [8] where also the residue method had been applied. Analogously to [6] the deviation was attributed to a failure of the saddle-point method, but is in fact due to the same unjustified omission of a non-vanishing integral. The direct applicability of the present findings to [8] can be verified, since the derivation in [8] differs from [6] essentially only by the choice of $\phi = \omega t$ as complex variable, while in [6] and the present work $u = \sin \omega t$ was used.

The applicability of the method of steepest descent (saddle-point approximation) for arbitrary ns states has also been investigated in the present work. It is found that the simple standard formula fails for large n . To overcome this problem a corrected formula is proposed.

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APPENDIX A: CALCULATION OF u_{\pm} , $S(u)$, $S'(u)$, $S''(u_{\pm})$, $S'''(u_{\pm})$, AND Q_{\pm} .

The integration of (11) for $|\mathbf{p}| = p_N$ yields

$$\exp[iS(u)] = \exp\left\{i\frac{\mathbf{p} \cdot \mathbf{F}}{\omega^2}[1 - f(u)] - i\frac{U_p}{\omega}uf(u)\right\} \times [f(u) + iu]^N. \quad (\text{A1})$$

For $u = Re^{i\theta}$ with $R \rightarrow \infty$, one has $f(u) \rightarrow -iu + iu^{-1}/2$ and

$$\exp[iS(u)] \rightarrow \frac{\exp\left\{-\frac{U_p}{\omega}u^2 - \frac{\mathbf{p} \cdot \mathbf{F}}{\omega^2}(u - i)\right\}}{(-2iu)^N}. \quad (\text{A2})$$

The saddle points u_{\pm} of $S(u)$ can be determined by the following condition:

$$\frac{E_b}{\omega} + \frac{1}{2\omega} \left(\mathbf{p} + \frac{\mathbf{F}}{\omega}u \right)^2 = 0. \quad (\text{A3})$$

Introducing the Keldysh parameter $\gamma = \kappa\omega/F$ with $\kappa = \sqrt{2E_b}$, the scaled momentum $\chi = p_N/\kappa$, and $\zeta = \hat{\mathbf{F}} \cdot \hat{\mathbf{p}}$

$$u_{\pm} = -\sigma \pm \rho i, \quad \sigma = \gamma\chi\zeta, \quad \rho = \gamma\sqrt{1 + \chi^2(1 - \zeta^2)} \quad (\text{A4})$$

is obtained. Using (A4) the first derivative $S'(u)$ can be expressed as

$$S'(u) = \frac{2U_p}{\omega} \frac{(u - u_+)(u - u_-)}{f(u)} \quad (\text{A5})$$

and the values of the second $S''(u)$ and third $S'''(u)$ derivatives at $u = u_{\pm}$ are given by

$$S''(u_{\pm}) = \pm \frac{4U_p\rho i}{\omega f(u_{\pm})}, \quad S'''(u_{\pm}) = \frac{6U_p - 2N\omega}{\omega f^3(u_{\pm})}. \quad (\text{A6})$$

The absolute value Q and the argument ϑ_s of Q_s defined by (21) can be written as

$$Q = \frac{\sqrt{2\omega\gamma}}{\sqrt{\rho\kappa}} [(1 + \sigma^2 + \rho^2)^2 - 4\sigma^2]^{1/8}, \quad (\text{A7})$$

$$\tan 4\vartheta_{\pm} = \pm \frac{2\sigma\rho}{1 + \rho^2 - \sigma^2}, \quad -\frac{\pi}{4} < \vartheta_{\pm} < \frac{\pi}{4}. \quad (\text{A8})$$

Note, for the small momentum limit $\mathbf{p} \ll \kappa$ the following relations are valid:

$$\rho \approx \gamma, \quad 1 - u_{\pm}^2 \approx 1 + \gamma^2 \pm 2\gamma^2\chi\zeta i, \quad (\text{A9})$$

$$Q \approx \frac{\sqrt{2\omega\gamma}}{\kappa} (1 + \gamma^2)^{1/4}, \quad \vartheta_{\pm} \approx \pm \frac{\chi\zeta\gamma^2}{2(1 + \gamma^2)}. \quad (\text{A10})$$

APPENDIX B: FUNCTION $\tilde{V}_0(u)$ FOR THE nS STATES OF A HYDROGEN-LIKE ATOM.

Consider the spherically symmetric state (with principal quantum number n) of a hydrogen-like atom with potential $U(\mathbf{r}) = Z/r$, where Z is the charge of the nucleus. Its Fourier transform is given by

$$\tilde{\Phi}_0(\mathbf{q}) = \frac{8\sqrt{\pi}}{\kappa^{3/2}} \sum_{k=0}^{n-1} (-1)^k 2^{2k} C_{2k+1}^{n+k} \left(\frac{\kappa^2}{\mathbf{q}^2 + \kappa^2} \right)^{k+2} \quad (\text{B1})$$

where C_k^n are binomial coefficients. Using the identity $\nabla_{\mathbf{q}} f(q^2) = 2\mathbf{q} \partial f(q^2) / (\partial q^2)$ one can rewrite Eq. (6) as

$$V_0(\mathbf{q}) = \frac{4\pi(\mathbf{F} \cdot \mathbf{q})}{\kappa F} \sum_{k=3}^{n+2} D_n^{(k)} \left(\frac{\kappa^2}{\mathbf{q}^2 + \kappa^2} \right)^k \quad (\text{B2})$$

where

$$D_n^{(k)} = (-1)^k (k-1) 2^{2k-4} C_{2k-5}^{n+k-3} \frac{iF}{\sqrt{\pi}\kappa^{5/2}}. \quad (\text{B3})$$

Introducing

$$P_{\pm}(u) = \frac{\gamma}{u - u_{\pm}} \quad (\text{B4})$$

and using

$$\mathbf{F} \cdot \mathbf{q} = \frac{F\kappa}{2} [P_+^{-1}(u) + P_-^{-1}(u)], \quad \frac{\kappa^2}{\mathbf{q}^2 + \kappa^2} = P_+(u)P_-(u),$$

one can rewrite Eq. (10) as

$$\tilde{V}_0(u) = \sum_{k=3}^{n+2} D_n^{(k)} \{P_+^{k-1}P_-^k + P_+^kP_-^{k-1}\}. \quad (\text{B5})$$

Introducing $R_{\pm} = P_{\pm}(u_{\mp}) = \mp\gamma/(2\rho i)$ and using the Taylor expansion of $P_{\pm}^k(u)$ at $u \approx u_{\mp}$,

$$P_{\pm}^k(u) = \sum_{m=0}^{\infty} (-1)^m C_m^{k+m-1} R_{\pm}^{k+m} P_{\mp}^{-m}(u), \quad (\text{B6})$$

one can rewrite $\tilde{V}_0(u)$ as a Laurent series at $u \approx u_{\pm}$

$$\tilde{V}_0(u) = \sum_{\nu=-\infty}^{n+2} \frac{M_{\pm}^{(n,\nu)}}{(u - u_{\pm})^{\nu}} \quad (\text{B7})$$

where

$$M_{\pm}^{(n,\nu)} = \gamma^{\nu} \sum_{r=\max(\nu,3)}^{n+2} D_n^{(r)} Q_{r-\nu}^{(r)} R_{\mp}^{2r-\nu-1}, \quad (\text{B8})$$

and

$$Q_m^{(k)} = (-1)^m \{C_m^{k+m-2} - C_{m-1}^{k+m-2}\}, \quad Q_0^{(k)} = 1. \quad (\text{B9})$$

Then for $g_{\pm}(u)$ defined in (13),

$$g_{\pm}(u) = \sum_{m=0}^{\infty} M_{\pm}^{(n,n+2-m)} (u - u_{\pm})^m, \quad (\text{B10})$$

one has

$$g_{\pm}(u_{\pm}) = M_{\pm}^{(n,n+2)} = (\pm 2)^{n-1} \frac{i^n (n+1) \gamma^{2n+3} F}{\sqrt{\pi} \rho^{n+1} \kappa^{5/2}}. \quad (\text{B11})$$

APPENDIX C: CORRECTED MSD FORMULA FOR THE nS STATES OF A HYDROGEN-LIKE ATOM.

Representing $\exp[iS(u)]$ as

$$\begin{aligned} \exp[iS(u)] &= \exp[iS(u) - (i/2)S''(u_s)(u - u_s)^2] \\ &\times \exp[-Q_s^2(u - u_s)^2] \end{aligned} \quad (\text{C1})$$

and performing a Taylor expansion of the first term on the right hand side of (C1) at $u = u_s$ yields

$$\begin{aligned} e^{iS(u)} &= e^{iS(u_s)} e^{-Q_s^2(u - u_s)^2} \\ &\times \left\{ 1 + \frac{iS'''(u_s)}{6} (u - u_s)^3 + \dots \right\}. \end{aligned} \quad (\text{C2})$$

Keeping the first two terms of the Taylor expansion the integrand in (9,16) can be rewritten as

$$\begin{aligned} \tilde{V}_0(u) e^{iS(u)} &\approx e^{iS(u_s)} e^{-Q_s^2(u - u_s)^2} \left\{ \sum_{\nu=-\infty}^{n+2} \frac{M_s^{(n,\nu)}}{(u - u_s)^{\nu}} \right. \\ &\left. + \frac{iS'''(u_s)}{6} \sum_{\nu=-\infty}^{n-1} \frac{M_s^{(n,\nu+3)}}{(u - u_s)^{\nu}} \right\}. \end{aligned} \quad (\text{C3})$$

Omitting terms with negative ν in (C3) and applying the procedure described in Sec. II D

$$\begin{aligned} I_{s;cMSD}^{\pm} &= \pi e^{iS(u_s)} \left\{ \sum_{\nu=0}^{n+2} \frac{(\pm 1)^{\nu} M_s^{(n,\nu)}}{i^{\nu} Q_s^{\nu-1} \Gamma(\frac{\nu+1}{2})} \right. \\ &\left. + \frac{iS'''(u_s)}{6} \sum_{\nu=0}^{n-1} \frac{(\pm 1)^{\nu} M_s^{(n,\nu+3)}}{i^{\nu} Q_s^{\nu-1} \Gamma(\frac{\nu+1}{2})} \right\} \end{aligned} \quad (\text{C4})$$

is obtained as approximation for I_s^{\pm} . Note, that neglecting all terms with $\nu < n+2$ in (C4) and using (B11) one obtains the simple (standard) MSD formula (29) for I_s^{\pm} . A corrected approximation for $A(\mathbf{p})$ is then obtained using (22) as

$$A_{cMSD} = I_{+;cMSD}^{-} - I_{-;cMSD}^{+}. \quad (\text{C5})$$

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